Development of Thermodynamic Properties of Electrolyte Solutions with the Help of RISM-Calculations at Born-Oppenheimer Level

Electronic Supplementary Information

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Tables of computed values of the chemical excess potential

		DRISM			RISM			
		Na^+	Cl^-	NaCl	H_2O	Na^+	Cl^-	NaCl
$c/mol\,dm^{-3}$	$sqrt(\Gamma)$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}_{\pm}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}_{\pm}$
0.000	0.000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
$9.00 \cdot 10^{-8}$	$4.243 \cdot 10^{-4}$	-0.0038	-0.0041	-0.0040	0.0000	-0.0156	-0.0163	-0.0159
$2.60 \cdot 10^{-5}$	$7.213 \cdot 10^{-3}$	-0.0059	-0.0059	-0.0059	0.0001	-0.0749	-0.0758	-0.0753
$9.00 \cdot 10^{-4}$	$4.243 \cdot 10^{-2}$	-0.0476	-0.0442	-0.0459	0.0025	-0.6227	-0.6258	-0.6243
$4.20 \cdot 10^{-3}$	$9.165 \cdot 10^{-2}$	-0.1110	-0.1155	-0.1132	0.0121	-1.2575	-1.2735	-1.2655
$6.40 \cdot 10^{-3}$	$1.131 \cdot 10^{-1}$	-0.1384	-0.1492	-0.1438	0.0185	-1.5160	-1.5406	-1.5283
$1.00 \cdot 10^{-2}$	$1.414 \cdot 10^{-1}$	-0.1751	-0.1966	-0.1859	0.0289	-1.8437	-1.8822	-1.8629
$1.44 \cdot 10^{-2}$	$1.697 \cdot 10^{-1}$	-0.2130	-0.2477	-0.2303	0.0416	-2.1588	-2.2144	-2.1866
$1.96 \cdot 10^{-2}$	$1.980 \cdot 10^{-1}$	-0.2522	-0.3026	-0.2774	0.0566	-2.4630	-2.5387	-2.5008
$2.56 \cdot 10^{-2}$	$2.263 \cdot 10^{-1}$	-0.2927	-0.3617	-0.3272	0.0738	-2.7572	-2.8561	-2.8066
$3.24 \cdot 10^{-2}$	$2.546 \cdot 10^{-1}$	-0.3347	-0.4248	-0.3797	0.0933	-3.0424	-3.1674	-3.1049
$4.00 \cdot 10^{-2}$	$2.828 \cdot 10^{-1}$	-0.3781	-0.4929	-0.4355	0.1150	-3.3195	-3.4736	-3.3965
$\mu^{exc,\infty}$		-344.3420	-390.7078	-367.5299	-26.8897	-330.2414	-374.4850	-352.3637

Table 1: Twelve representative sets (out of 27) of the chemical potential of NaCl in water at 25°C at BO-level with HK-closure. All energies are given in $kJ\,mol^{-1}$. $\Delta\mu^{exc}$ is the difference of the chemical excess potential with respect to the extrapolated value at infinite dilution $\mu^{exc,\infty}$.

		RISM			
		H_2O	Na^+	NO_3^-	$NaNO_3$
$c/mol\,dm^{-3}$	$sqrt(\Gamma)$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}_{\pm}$
0.00	0.000	0.0000	0.0000	0.0000	0.0000
$9.00 \cdot 10^{-8}$	$4.243 \cdot 10^{-4}$	0.0000	-0.0170	-0.0014	-0.0092
$2.60 \cdot 10^{-5}$	$7.213 \cdot 10^{-3}$	0.0000	-0.0454	-0.0034	-0.0244
$9.00 \cdot 10^{-4}$	$4.243 \cdot 10^{-2}$	0.0023	-0.3926	-0.0308	-0.2117
$4.20 \cdot 10^{-3}$	$9.165 \cdot 10^{-2}$	0.0107	-0.7682	-0.0720	-0.4201
$6.40 \cdot 10^{-3}$	$1.131 \cdot 10^{-1}$	0.0163	-0.9168	-0.0925	-0.5046
$1.00 \cdot 10^{-2}$	$1.414 \cdot 10^{-1}$	0.0254	-1.1054	-0.1221	-0.6138
$1.44 \cdot 10^{-2}$	$1.697 \cdot 10^{-1}$	0.0367	-1.2887	-0.1547	-0.7218
$1.96 \cdot 10^{-2}$	$1.980 \cdot 10^{-1}$	0.0500	-1.4685	-0.1908	-0.8297
$2.56 \cdot 10^{-2}$	$2.263 \cdot 10^{-1}$	0.0653	-1.6461	-0.2300	-0.9380
$3.24 \cdot 10^{-2}$	$2.546 \cdot 10^{-1}$	0.0827	-1.8223	-0.2726	-1.0474
$4.00 \cdot 10^{-2}$	$2.828 \cdot 10^{-1}$	0.1023	-1.9979	-0.3187	-1.1583
$\mu^{exc,\infty}$		-26.8901	-330.2398	-111.5908	-220.9153

Table 2: Twelve representative sets (out of 27) of the chemical potential of $NaNO_3$ in water at 25°C at BO-level with HK-closure. All energies are given in $kJ\,mol^{-1}$. $\Delta\mu^{exc}$ is the difference of the chemical excess potential with respect to the extrapolated value at infinite dilution $\mu^{exc,\infty}$.

		RISM			
		H_2O	Me_4N^+	Cl^-	Me_4NCl
$c/mol\,dm^{-3}$	$sqrt(\Gamma)$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}_{\pm}$
0.00	0.00	0.0000	0.0000	0.0000	0.0000
$9.00 \cdot 10^{-8}$	$4.243 \cdot 10^{-4}$	0.0000	-0.0030	-0.0181	-0.0106
$2.60 \cdot 10^{-5}$	$7.213 \cdot 10^{-3}$	0.0002	-0.0058	-0.0470	-0.0264
$9.00 \cdot 10^{-4}$	$4.243 \cdot 10^{-2}$	0.0047	-0.0461	-0.4040	-0.2250
$4.20 \cdot 10^{-3}$	$9.165 \cdot 10^{-2}$	0.0219	-0.1184	-0.8052	-0.4618
$6.40 \cdot 10^{-3}$	$1.131 \cdot 10^{-1}$	0.0334	-0.1567	-0.9690	-0.5629
$1.00 \cdot 10^{-2}$	$1.414 \cdot 10^{-1}$	0.0522	-0.2133	-1.1813	-0.6973
$1.44 \cdot 10^{-2}$	$1.697 \cdot 10^{-1}$	0.0752	-0.2771	-1.3923	-0.8347
$1.96 \cdot 10^{-2}$	$1.980 \cdot 10^{-1}$	0.1024	-0.3483	-1.6040	-0.9761
$2.56 \cdot 10^{-2}$	$2.263 \cdot 10^{-1}$	0.1338	-0.4272	-1.8175	-1.1224
$3.24 \cdot 10^{-2}$	$2.546 \cdot 10^{-1}$	0.1695	-0.5140	-2.0338	-1.2739
$4.00 \cdot 10^{-2}$	$2.828 \cdot 10^{-1}$	0.2095	-0.6086	-2.2537	-1.4312
$\mu^{exc,\infty}$		-26.8902	-61.3004	-374.4790	-217.8899

Table 3: Twelve representative sets (out of 27) of the chemical potential of Me_4NCl in water at 25°C at BO-level with HK-closure. All energies are given in kJ mol^{-1}. $\Delta\mu^{exc}$ is the difference of the chemical excess potential with respect to the extrapolated value at infinite dilution $\mu^{exc,\infty}$.

		RISM-HNC		
		Na^+	Cl^-	NaCl
$c/mol\,dm^{-3}$	$sqrt(\Gamma)$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}$	$\Delta\mu^{exc}_{\pm}$
0.00	0.000	0.000	0.000	0.000
$9.00 \cdot 10^{-8}$	$4.243 \cdot 10^{-4}$	-3.826	-3.902	-3.864
$2.60 \cdot 10^{-5}$	$7.213 \cdot 10^{-3}$	-3.912	-3.989	-3.950
$9.00 \cdot 10^{-4}$	$4.243 \cdot 10^{-2}$	-6.553	-6.660	-6.606
$4.20 \cdot 10^{-3}$	$9.165 \cdot 10^{-2}$	-14.229	-14.493	-14.334
$6.40 \cdot 10^{-3}$	$1.131 \cdot 10^{-1}$	-18.119	-18.390	-18.254
$1.00 \cdot 10^{-2}$	$1.414 \cdot 10^{-1}$	-23.252	-23.614	-23.443
$1.44 \cdot 10^{-2}$	$1.697 \cdot 10^{-1}$	-28.421	-28.887	-28.654
$1.96 \cdot 10^{-2}$	$1.980 \cdot 10^{-1}$	-34.459	-35.054	-34.756
$\mu^{exc,\infty}$		-349.098	-388.788	-368.943

Table 4: Nine representative sets (out of 24) of the chemical potential of NaCl in water at 25°C at RISM-BO-level with HNC-closure. All energies are given in kJ mol^{-1}. $\Delta\mu^{exc}$ is the difference of the chemical excess potential with respect to the extrapolated value at infinite dilution $\mu^{exc,\infty}$